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HOLISTIC MESOSCALE MODELLING OF CONCRETE – RECENT DEVELOPMENTS

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Abstract. Modelling of concrete at the mesoscale is needed in many applications, but developing a realistic mesoscale model for the analysis of concrete behaviour under general loading conditions is challenging. This paper presents an overview of the development of mesoscale modelling of concrete within a finite element framework for both quasi-static and high strain rate applications. A 2D mesoscale model incorporating random aggregates and equivalent interfacial transition zones enables examination into the effects of random aggregate structure and the sub-scale non-homogeneity within the mortar matrix on the macroscopic behaviour of concrete. In applications where multi-axial stresses and confinement effects are significant, such as under high-strain rate loading where the inertial confinement plays an important role, a realistic representation of the multi-axial stress condition becomes necessary, and this requires 3D mesoscale model. Two types of 3D mesoscale concrete model have been developed, namely a pseudo-3D mesoscale model and a full 3D mesoscale model. For the explicit representation of the fracture process, a cohesive-contact approach has been implemented, at present in a 2D mesoscale framework. Illustrative examples are given to demonstrate the performance of the mesoscale models and the results are discussed.

1 INTRODUCTION

The behaviour of concrete has a strong influence by the composition of the concrete mix and the process of damage and fracture within the mortar matrix and at the interfacial transition zone (ITZ). To capture the underlining damage process requires appropriate representation of the material composition and this means a mesoscale model. In fact modelling of concrete at the mesoscale is needed in many applications, for example for investigation into the micro-meso mechanics underlying the macroscopic behaviour of the concrete material, and for realistic simulation of damage evolution in critical regions of concrete structures where complex stress conditions take place.

In standard computational modelling of concrete structures, concrete is typically modelled as homogeneous material with macroscopic material properties. Such an approach is computationally economical, and can be suited for a wide range of applications. However, the constitutive laws in homogenised models for concrete are derived from the nominal stress-strain response of standard specimens, therefore the applicability of the macroscopic model are generally limited to problems which does not involve drastic spatial variation of the stress and strain within a certain characteristic dimension. For an analysis where finer spatial resolution than the characteristic size of bulk concrete or representative volume element RVE is required, homogenization can no longer be justified. It is clear that the properties of the material would exhibit a much increased scatter as the element size is reduced into the sub-RVE regime [1].

For a conceptual discussion, four levels of spatial discretization may be defined for the purpose of classifying the material descriptions [2], as schematically illustrated in Fig. 2. Spatial discretization at levels I and II may be suitable mainly in quasi-static loading analysis and for relatively large structures, and homogenization is most appropriate for these levels of discretization. On the other hand, for problems such as high strain rate loading, spatial discretization at levels III and IV are commonly used due to the need of capturing the transient stress wave effects. As the discretization refines, the properties of the material within individual elements will tend to vary distinctively, and eventually resembles the variation in a mesoscale framework, i.e. between mortar and aggregates.

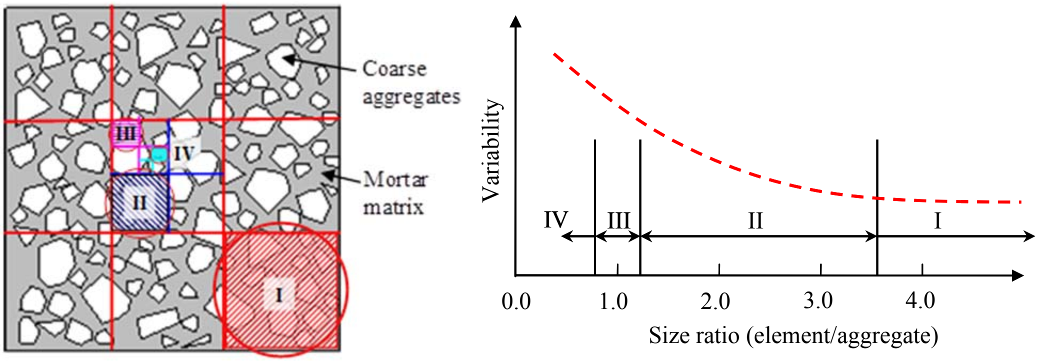


Figure 1: Representative levels of discretization (left) and variability of material properties (right) [2]

Modelling of concrete at the mesoscale has been a subject of much research over the last 3 decades. Three main alternative approaches have been employed, namely lattice models (e.g. [3]), discrete element models (e.g. [4-5]), and continuum based FE models. A main challenge with the lattice models is the difficulty in determining the equivalent model parameters. Similar issues exist in the DEM approach where the interface between aggregates and the mortar matrix, which effectively is continuous, has to be represented through contacts. The determination of the modelling parameters in a continuum based FE model, on the other hand, is relatively more straightforward.

Mesoscale modelling of concrete using a continuum-based finite element framework allows for the multi-phasic continuous nature of concrete to be explicitly represented. The evolving discontinuity due to fracture can be simulated by damage laws of the constituent materials. Most of the early mesoscale models were actually developed in this framework (e.g. [6-8]). However, Generation of the meso-geometry and the FE meshing are the main challenges. Especially for 3-dimensional (3D) mesoscale models, simplified geometries with spherical or elliptical inclusions are often employed, while alternative methods include the use of regular FE method and create the heterogeneity by joining adjacent elements to form aggregates (e.g. [9]).

A series of studies has been undertaken in recent years by the authors and co-workers in developing a holistic mesoscale modelling framework for general analysis of concrete under a variety of loading conditions. A 2D mesoscale model incorporating random aggregates and equivalent interfacial transition zones enables examination into the effects of random aggregate structure and the sub-scale non-homogeneity within the mortar matrix on the macroscopic behaviour of concrete. In applications where multi-axial stresses and confinement effects are significant, including high-strain rate loading where the inertial confinement plays an important role, a realistic representation of the multi-axial stress condition becomes necessary, and this requires 3D mesoscale model. Two types of 3D mesoscale concrete model have been developed, namely a pseudo-3D mesoscale model and a full 3D mesoscale model. In the latest development, a cohesive-contact approach has been adopted in the description of the ITZ to allow for explicit representation of complex fracture and interaction between fractured surfaces. This approach has been implemented in a 2D mesoscale framework and work is to be carried out to extend this approach to 3D mesoscale analysis.

2 THE GENERAL 2D MESOSCALE MODEL

The creation of a 2D (as well as 3D) mesoscale model for concrete starts with the generation of the random geometric structure encompassing random polygon (or polytope) aggregates following a specified size distribution, e.g., a Fuller curve. A standard take-and-place procedure is employed in which individual aggregates are randomly generated and placed into the space representing the target concrete specimen. Checks are carried out to ensure that aggregates do not overlap and that a minimum gap is preserved between aggregates. Once a target packing density (defined by the volume ratio of the aggregates) is satisfied, the geometric structure creation phase is completed and the geometric data are taken to a mesh generator for meshing. Fig. 2 depicts a sample of the generated mesoscale geometry and the FE mesh for the three individual phases. Note that the ITZ phase here is represented by an equivalent thin layer of solid elements in the model shown.

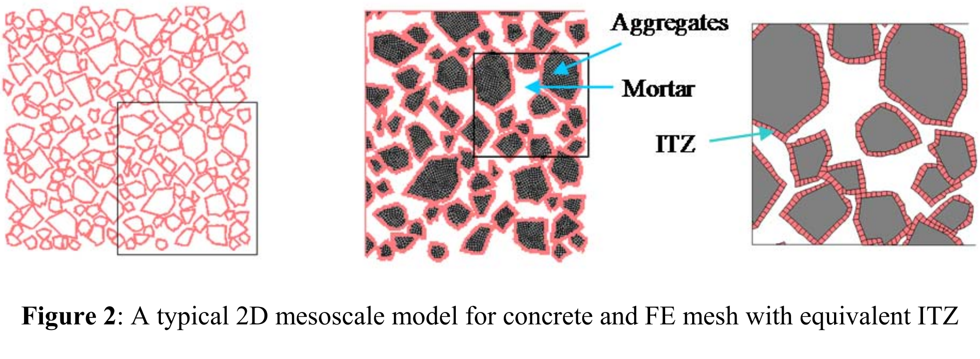
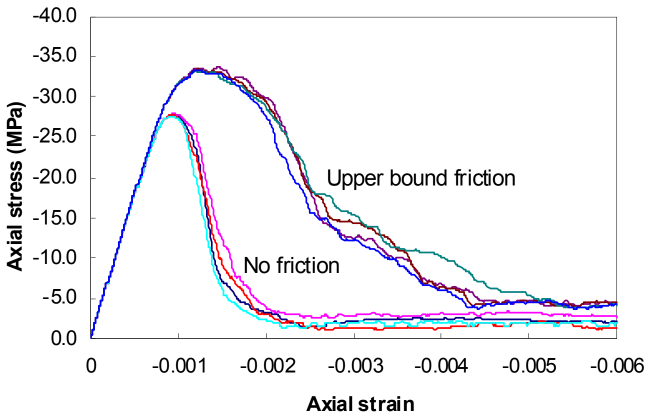


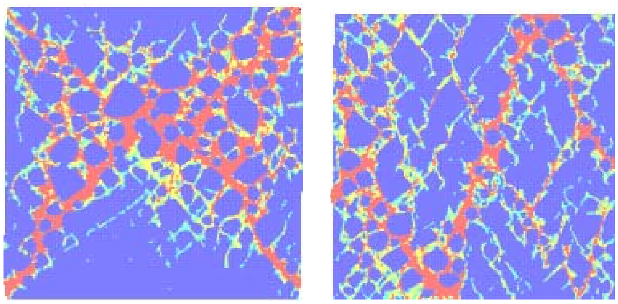
Figure 2: A typical 2D mesoscale model for concrete and FE mesh with equivalent ITZ

The material models for aggregates and mortar matrix can be adapted to represent the specific properties for these distinctive materials. For quasi-static loading aggregates do not normally fail and so use may be made of elastic material model for aggregates. For mortar matrix a generic geomaterial constitutive model may be appropriate, and in the present study we use the concrete damage model (K&C model [10]) which is available in LS-DYNA, the software utilised to carry out the mesoscale model analysis in the present study.

It is worth noting that further variability of the material properties within each of the three individual phases may be incorporated by a stochastic sampling approach such that each element will acquire a specific property from a target property distribution. Fig. 4 shows a set of simulated cubic compressive stress-strain curves for 30-MPa concrete using the 2D mesoscale model. The variation in the post-peak regime reflects the influence of varying the material properties within each individual phase.



(a) Stress-strain curves: variation in descending branch attributable to random properties within each material



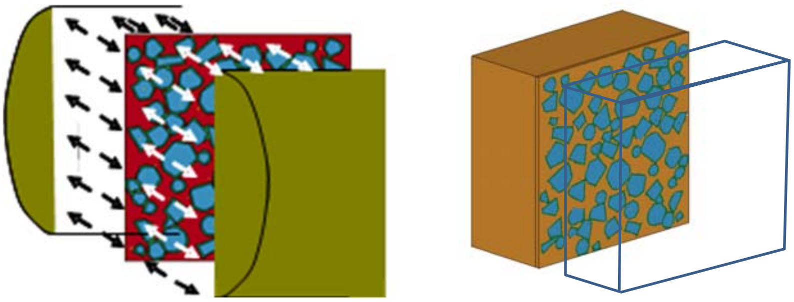
(b) Damage patterns: High friction (left) and Low friction (right)

Figure 3: Computed compressive stress-strain curves for 30-MPa concrete for two levels of loading face frictions and the damage patterns

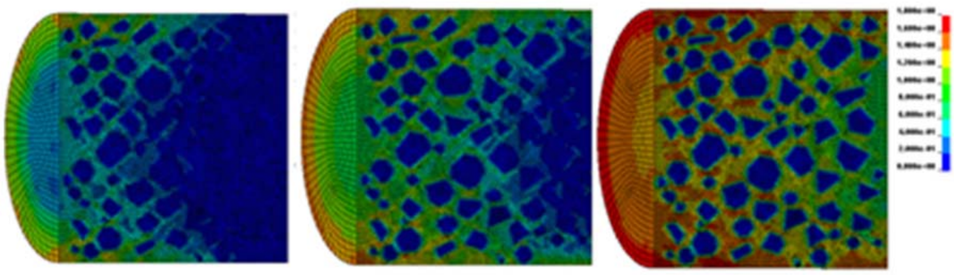
3 A PSEUDO 3D MESOSCALE MODEL

For concrete under multi-axial stresses, a 3D mesoscale model would be desirable, which however means significantly increased computational cost. As an alternative to a true 3D mesoscale model, a pseudo 3D mesoscale model has been devised. Fig. 4 illustrates such a pseudo 3D mesoscale scheme. The actual mesoscale description is contained in a slice of 2D mesoscale model, in which the mesoscale features are fully represented. The 3D effect is achieved by sandwiching the mesoscale layer between two half-sized homogeneous bodies to complete the whole specimen. The interface between the mesoscale layer and the homogeneous parts is made to be friction free but fully coupled in the normal direction, so that any incompatibility within the mesoscale plane will have no effect on the mesoscale model part while transmission of the pressure (confining stress) on the mesoscale model is almost fully preserved.

A schematic of the pseudo 3D mesoscale model setup for cylinder and cube specimens is given in Fig. 4(a). Fig. 4(b) shows the effects of the model in creating a realistic 3D stress field for the mesoscopic observations.



(a) Model setup: cylinder (left) and cube (right) specimens



(b) Pseudo 3D cylinder under fast compression: 3D stress field is clearly visible

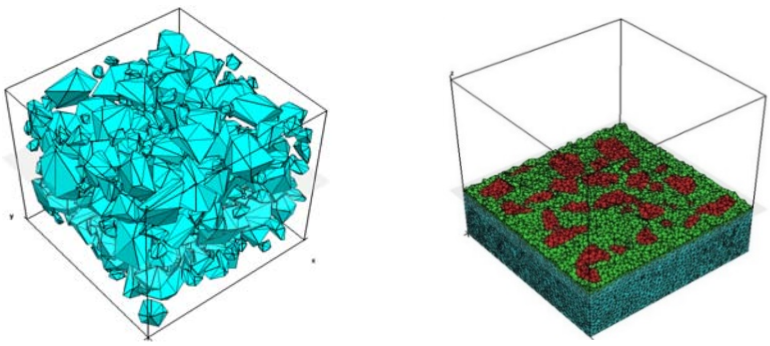
Figure 4: Pseudo 3D mesoscale models and simulation effects [11]

4 A FULL 3D MESOSCALE MODEL

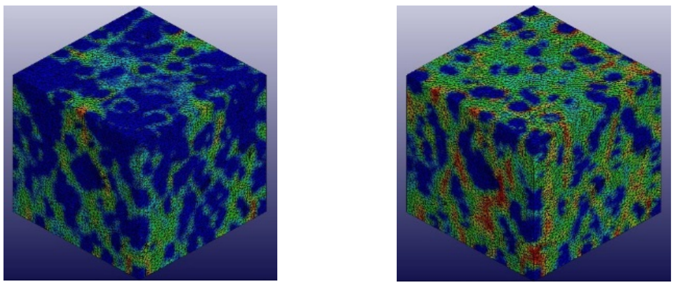
For a fuller description of the 3D mesoscale structure and the associated 3D effects, especially under high strain rate loading, a true 3D mesoscale model with random polytopes has also been developed. The procedure of creating such a 3D mesoscale model is similar to the 2D mesoscale model, but the complexities in the generation of the random mesoscale geometry increase. In the present scheme, we create the aggregate particles by bounded polyhedrons in convex hulls according to computational geometry. Flaky and elongated aggregates are realised from the regular polytopes by shrinking or elongation operations. In the subsequent 'place' process, a pre-selection algorithm is used to identify the existing polytopes that may have a chance to intersect with the one being placed. Subsequent intersection check only needs to be carried out for polytopes whose bounding spheres intersect with that of the current particle. To improve the efficiency of the existing "place" procedure, in the event an aggregate being placed is found to intersect with any aggregates already in place, a translate-and-rotate procedure is employed on the aggregate being placed.

Fig. 5(a) shows a typical 3D mesoscale aggregate structure. The remaining space in the sample domain is automatically occupied by the mortar matrix, while the interface between the aggregates and the mortar matrix may be treated as the ITZ. It should be mentioned that meshing for a 3D mesoscale model in not a trivial task. Due to randomly shaped aggregates, the meso-structure is highly unstructured. Specific smoothing algorithms such as Octree, advancing front and Delaunay refinement need be involved for meshing unstructured domain. Fig. 5(a) also shows an example of the 3D FE mesh. In the model shown the interface in treated an equivalent thin layer of solid elements surrounding the aggregates.

The 3D mesoscale model can then be subjected to any loading by applying appropriate boundary conditions. Fig. 5(b) shows an example analysis under high rate compression with a nominal strain rate at 50 s^{-1}, The phenomenon of distributed damage and the 3D inertia confinement effect is clearly reproduced in a the 3D mesoscale model.



(a) A full 3D mesoscale model: meso-geometry



(b) Pseudo 3D cylinder under high rate compression

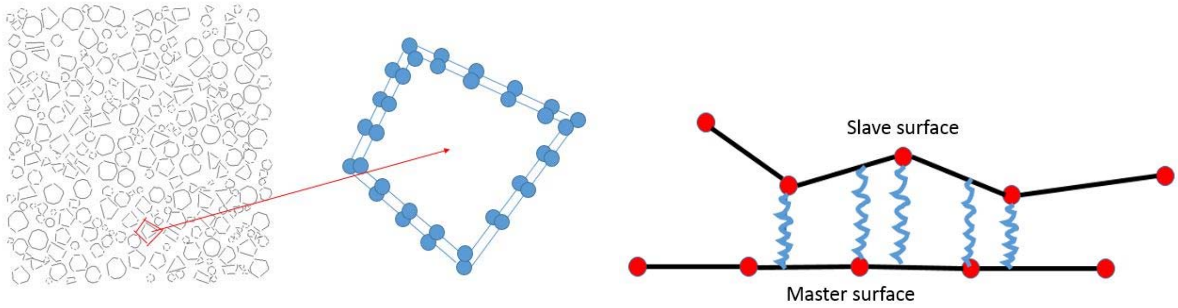
Figure 5: 3D mesoscale model and example simulation

5 A COHESIVE-CONTACT INTERFACE MODEL FOR THE ITZ

In the above-described mesoscale models, fracture within the material is generally represented by failure of the corresponding solid elements through the constitutive descriptions. Although the effect of fracture can be reproduced to a large extent through the deterioration and loss of strength and stiffness in the elements, the inability of depicting explicitly the discontinuity induced by fractures limits the capability of the model in replicating the fracture evolution, and fracture opening and closure processes.

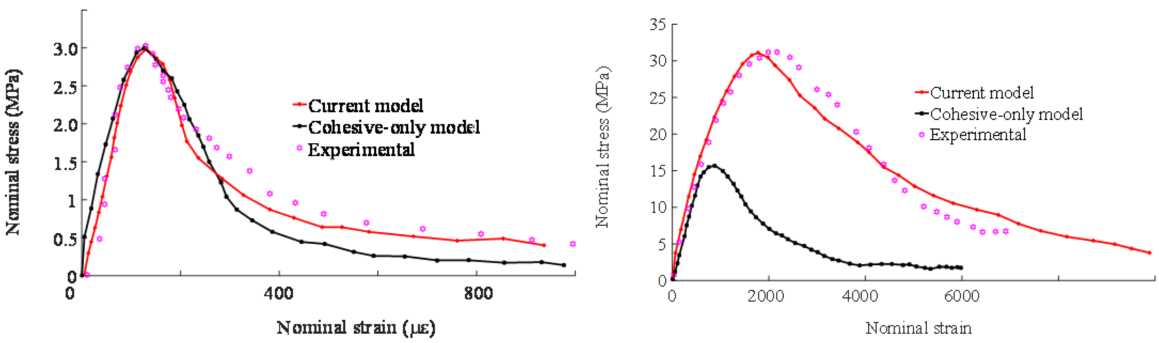
To tackle this issue a cohesive-contact model has been incorporated in a mesoscale framework. The incorporation of the contact process is to address the problem with the classical cohesive model in which complex stress condition at the interface is often ignored or treated poorly, resulting in poor performance of the model under general loading other than simple tension or shear ([12]).

Fig. 6 depicts the generation of the zero-thickness interface elements for the ITZ in the mesoscale model, and Fig. 7 shows the simulated stress-strain curves under uniaxial tension and compression using such a mesoscale model. It is clearly observed that, while the new interface model maintains similar effect as the cohesive-only model in a tension condition, significant improvement is achieved under compression. As the interface is always subjected to complex stress conditions in a mesoscale model even though the whole specimen is under a uniaxial loading, the satisfactory performance of the cohesive-contact approach indicates that this approach is effective in practically any interface stress conditions.



(a) Generation of interface element (b) Incorporation of contact in interface element

Figure 6: Interface elements with cohesive and contact-friction functions



(a) Uniaxial tension (b) Uniaxial compression

Figure 7: Simulation of uniaxial tension and compression with the cohesive-contact mesoscale model

At present the cohesive-contact modelling approach has been implemented in 2D mesoscale models. The extension to general 3D mesoscale will clearly incur significant increase in the computation cost but in principle it is doable.

6 CONCLUSIONS

A series of studies has been undertaking to develop a holistic mesoscale modelling framework for numerical simulation of concrete and concrete-like materials under general loading and stress conditions. The mesoscale model in 2D allows realistic representation of the material composition and is suitable for characterisation of the mesoscopic damage processes and quantitative simulation of the concrete behaviour under uniaxial and biaxial stress conditions. The incorporation of the cohesive-contact interface for the ITZ enables explicit simulation of the fracture and the induced discontinuity, and therefore allows for direct simulation of complex processes involving discontinuity such as cyclic process of crack opening and closure, as well as shear interlock.

The development of the 3D mesoscale models allows simulation of loadings in which significant pressure (hydrostatic stress) component is involved, such as confined concrete, and concrete under high strain rate compression where lateral inertia confinement is known to play a significant role.

The mesoscale modelling approach can be employed to assist in the material investigation, characterisation, and the analysis of concrete structures in critical regions where the true behaviour of the material has so far been understood on a largely empirical basis.

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